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Authors
Brown, Christopher
Chen, Junjie

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Homogeneous charge compression ignition of fuel-lean methane-air mixtures over alumina-supported platinum catalysts in small-scale free-piston engines

Christopher Brown [a], Junjie Chen [a, b, c, *]

[a] Department of Mechanical and Aerospace Engineering, College of Engineering, University of California, Davis, California, 95616, United States

[b] Department of Automotive Engineering, School of Mechanical and Automotive Engineering, South China University of Technology, Guangzhou, Guangdong, 510641, P.R. China

[c] Department of Energy and Power Engineering, School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo, Henan, 454000, P.R. China

* Corresponding author. E-mail address: junjiem@tom.com

Abstract

The heterogeneous and homogeneous combustion-based homogeneous charge compression ignition of fuel-lean methane-air mixtures over alumina-supported platinum catalysts was investigated experimentally and numerically in free-piston micro-engines without ignition sources. Single-shot experiments were carried out in the purely homogeneous and coupled heterogeneous and homogeneous combustion modes, involved temperature measurements, capturing the visible combustion image sequences, exhaust gas analysis, and the physicochemical characterization of catalysts. Simulations were performed with a two-dimensional transient model that includes detailed heterogeneous and homogeneous chemistry and transport, leakage, and free-piston motion to gain physical insight and to explore the heterogeneous and homogeneous combustion characteristics. The micro-engine performance concerning combustion efficiency, mass loss, energy density, and free-piston dynamics was investigated. The results reveal that heterogeneous reactions cause earlier ignition, which is very favourable for the micro-device. Both purely homogeneous and coupled heterogeneous and homogeneous combustion of methane-air mixtures in a narrow cylinder with a diameter of 3 mm and a height of approximately 0.3 mm are possible. Heat losses result in higher mass losses. The coupled heterogeneous and homogeneous mode can not only significantly improve the combustion efficiency, in-cylinder temperature and pressure, output power and energy density, but also reduce the mass loss because of its lower compression ratio and less time spent around the top dead centre and during the expansion stroke, indicating that this coupled mode is a promising combustion scheme for micro-engines.

Keywords: Micro-engines; Homogeneous combustion; Free-piston dynamics; Power generation; Transient models; Micro-combustion

1. Introduction

Recently, micro-scale combustion has attracted increased attention because of the growing interest in developing portable power generation systems, with increasing efforts toward miniaturizing thermal engines for electricity production of a few tens of Watts [1]. Specifically, the high energy density of hydrocarbon fuels allows for the realization of micro-scale power generation systems [2]. Among the micro-scale system using the chemical energy of hydrocarbon fuels, micro-scale heat engine is being explored [3]. Micro-engine-based power supplies can deliver large energy density, and may eventually replace traditional lithium-ion batteries in various applications [4].

How to prevent thermal and radical quenching and achieve stable combustion is one of the most challenging issues to the micro-engine designer. Quenching is a matter of great concern because the specific heat transfer rate varies inversely with the characteristic dimension of the combustion chamber [5]. As engine size decreases, the surface-to-volume ratio increases, resulting in increased heat losses and increased potential destructions of active radicals on the combustion chamber walls. These mechanisms will increase the chemical reaction time and possibly inhibit the onset of homogeneous ignition, resulting in thermal or radical quenching [6]. Another concern is residence time, decreasing the dimension of the combustion chamber results in significant reduction of residence time because the flow velocity cannot be reduced accordingly. Insufficient residence time results in partial or incomplete combustion, in turn resulting in insufficient heat generation and further quenching [7]. In micro-scales, traditional engine combustion schemes are generally infeasible because of quenching effects and insufficient residence times. When considering micro-scale application, HCCI combustion mode is a promising alternative because it has the following experimentally verified characteristics: ignition is not initiated by an external event; the charge is consumed very rapidly; ignition occurs simultaneously at numerous locations inside the combustion chamber; and an absence of traditional flame propagation [8]. In the context of micro-combustion, the fundamental attributes of homogeneous charge compression ignition combustion are that an external ignition system is not required, and that the charge is combusted essentially without flame propagation. In addition, auto-ignition suggests that the charge is consumed both uniformly and rapidly, consequently minimizing quenching effects and without resorting to complicated ignition schemes. This concept may be a way toward elimination of ignition sources from micro-scale devices, resulting in further reduction of system size [9]. Additionally, homogeneous charge compression ignition combustion rate limited by chemical kinetics rather than transport and essentially no flame propagation result in shorter charge consumption time and in turn higher engine speed and efficiency [10]. These traits essentially bring HCCI combustion closer to a constant volume procedure, pushing the thermodynamic process closer to an ideal Otto cycle [11]. Furthermore, the ability to sustain homogeneous combustion with very lean mixtures reduces fuel mass losses through the leakage between the cylinder and piston, adversely enhancing fuel consumption efficiency [10, 11].

However, homogeneous charge compression ignition engines are more difficult to control than traditional engines. The combustion occurrence depends on chemical kinetics and the compression process [12, 13]. Therefore, controlling ignition timing is a challenge because it must be done indirectly. Experiments have demonstrated that employing a variable compression ratio is a promising approach to control homogeneous charge compression ignition [9]. Therefore, to utilize this strategy, an untraditional engine such as a free-piston engine is necessary, and is a very promising homogeneous charge compression ignition engine concept due to its valuable feature of variable compression ratio. The distinguishing feature of this device is a mechanically unconstrained free-piston; the free-piston motion is not restricted by a crankshaft mechanism, but is completely determined by gas pressure forces. In addition, the free-piston engine is a promising power generation device, offering the benefits of higher thermal efficiency and heat release rate compared to those of the traditional engine [14], extensive operation optimization [15], mechanical simplicity [16], multi-fuel combustion mode flexibility [17], and reduced nitrogen oxides formation [18, 19].

Computational models for simulating combustion and heat transfer of homogeneous charge compression ignition engines require detailed chemistry models; this is primarily because the ignition of homogeneous charge compression ignition engines is more sensitive to chemical kinetics. In addition, computational models have demonstrated that the importance of accounting for the fact that the in-cylinder mixture is actually in-homogeneous, particularly in terms of temperature field [20]. This in-homogeneity is driven by heat transfer from the combustion chamber walls and the turbulent mixing of fuel. Moreover, recent simulations have demonstrated that the charge inhomogeneity has a significant effect on the pressure rise rates and the consequential engine performance [21, 22]. The charge in-homogeneity would increase with decreasing cylinder size because in-homogeneities in the cylinder is caused by the thermal boundary layer adjacent to the cylinder walls [20]. The increased charge in-homogeneity, coupled with the high surface-area-to-volume ratio, may ultimately constrain the combustion chamber dimension. Furthermore, homogeneous combustion is mainly controlled by the temperature boundary layer and reactant species profiles [23, 24]. Consequently, in this work, a spatial dimensionality of at least two is necessary to correctly describe interphase transport and homogeneous combustion in particular.

The present work undertakes a combined experimental and numerical investigation of the heterogeneous and homogeneous combustion-based homogeneous charge compression ignition of fuel-lean methane-air mixtures over alumina-supported platinum catalysts in a free-piston micro-engine, which is candidate for small portable power generation applications. Single-shot experiments in the purely homogeneous and coupled heterogeneous and homogeneous combustion modes were performed in a free-piston micro-engine with a cylinder bore of 3 mm, involved temperature measurements, capturing the visible heterogeneous and homogeneous combustions image sequences, exhaust gas analysis, and physicochemical characterization of catalysts. A two-dimensional transient numerical model incorporating detailed heterogeneous and homogeneous chemistry and transport, leakage, dynamic mesh, turbulence, and thermodynamic-dynamic balance is developed to interpret the single-shot experimental results as well as to explore heterogeneous and homogeneous combustion characteristics. Following numerical validation and interpretation of the single-shot experimental results, the transient model was used to investigate the purely homogeneous and coupled heterogeneous and homogeneous combustion characteristics. In addition, the performance of free-piston micro-engines with regard to fuel conversion efficiency and mass loss was investigated. The primary objective of this work is to explore the feasibility of coupled heterogeneous and homogeneous combustion-based homogeneous charge compression ignition in free-piston micro-engines, and to characterize the purely homogeneous and coupled heterogeneous and homogeneous combustion at the micro-scale as well as to explore the free-piston dynamics. Of particular interest in the present work is to resolve the poor power density and low fuel conversion efficiency caused by exceedingly short charge consumption time and flow residence time as a result of extremely high free-piston oscillation frequency in free-piston micro-engines.

2. Experimental methods

Single-shot experiments were performed to characterize heterogeneous and homogeneous combustion at the micro-scale, as well as to explore the free-piston dynamics. The experimental setup used consists of a single-shot micro-engine designed to reproduce one compression-combustion-expansion cycle of the continuous process. This allows for very good control of the initial fuel-air mixtures in the combustion chamber by avoiding the detrimental effect of products remaining in the combustion chamber from previous cycles; it also ensures that other process parameters are the same for each experiment. The heterogeneous and homogeneous combustion experiments at the micro-scale are illustrated schematically in Figure 1 and the general principle is equally simple. A free-piston is driven into a visual cylinder filled with the combustible mixtures, while digital movies and thermal image of the total heterogeneous and homogeneous combustion process are achieved. The digital movies capture visible combustions and provide temporal measurements of velocity and position of the free-piston. Gas chromatography provided the exhaust composition, whereas infrared thermal imager was used to measure the two-dimensional temperature distributions inside the combustion chamber. Additionally, since the high surface to volume ratio of miniature internal combustion engine, the friction between the cylinder walls and the sealing rings become a major factor, and in some cases are in the order of the power of miniature engine. For this reason, no rings are practically installed in these miniature engines [10]. Therefore, to minimize the piston-cylinder walls gap, high precision manufacturing is required. In these miniature engines, the charge leakage is therefore unavoidable, and consequently high engine speed is required to reduce the mass losses incurred [11].

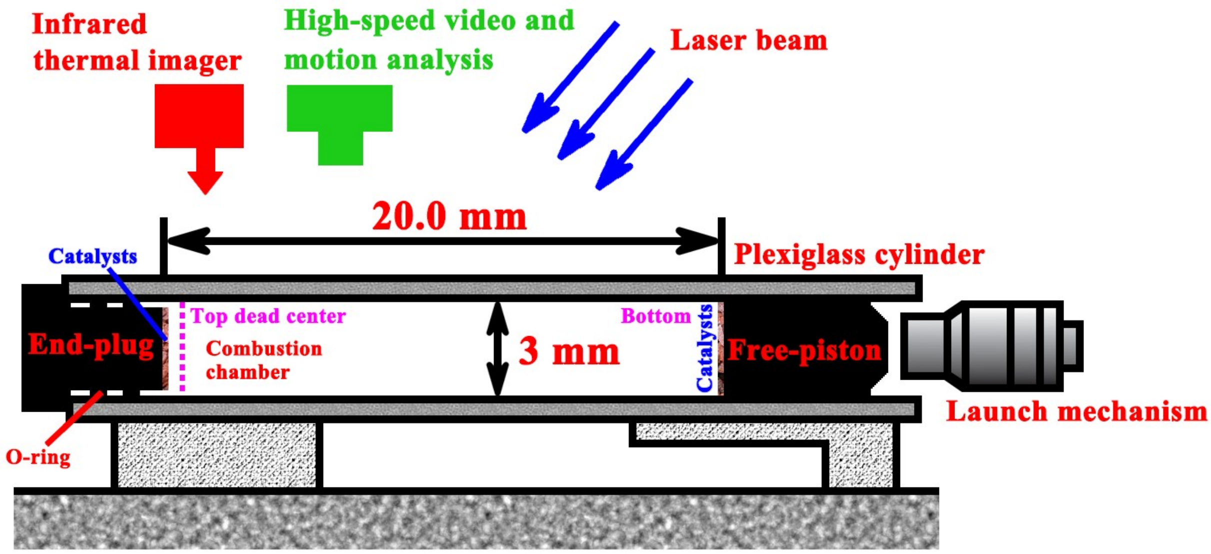


Figure 1. Schematic representation of the single-shot experiment. A free-piston is driven into a visual cylinder filled with the combustible mixtures, while digital movies and thermal image of the total heterogeneous and homogeneous combustion process are achieved.

Movement of the free-piston is initiated by injection of compressed air through the launch mechanism, consequently the launch mechanism with an extremely high velocity impulses the free-piston. The visual cylinder made with plexiglass that has good pressure-resistance and heat-resistance performance is initially filled with the methane-air homogenous mixtures, then the free-piston compresses the charge until it self-combusts. The free-piston and end-plug is ferrochrome-alloy, and the upper surface of the free-piston and the lower surface of the end-plug were coated with a catalyst, as shown in Figure 1. The initial distance between free-piston and end-plug, which is the chamber length, is 20.0 mm and the cylinder is sealed by a stainless-steel end-plug and two O-rings. The free-piston is a machined stainless steel gauge pin, having a mass of 0.5 g. The free-piston is 2.997 mm in diameter with an accuracy of 0.003 mm. Nominally, the inside diameter of the plexiglass cylinders is 3 mm. However, the actual dimensions of these plexiglass cylinders vary considerably. Therefore, fit-tests are used to match the free-piston to these plexiglass cylinders. The optimum cylinder and free-piston combination occurs when the outside diameter of the free-piston and the inside diameter of the cylinder differ by approximately 0.006 mm. In order to ensure that the free-piston is not easy to be distorted and damaged and the intensity is high when operating at high temperatures, quenching treatment of the free-piston is used to improve the surface capability. Furthermore, the free-piston surface is coated with nickel, which is prepared by electroplating, resulting in a high surface flatness and a decrease in the friction energy loss between the cylinder walls and the free-piston. As a result, the fit precision and sealing performance of combustion chamber is improved. In addition, the free-piston is lubricated to improve sealing performance. Although these methods ensure that the free-piston engine has excellent air tightness at ambient temperature and pressure, high in-cylinder pressure and temperature can aggravate the situation. As a result, most of the mass loss occurs around the top dead center, as will be discussed in the combustion characteristics section. Therefore, the gas tightness detection can hardly be achieved today, and it is still a challenging and interesting task for the future.

Such an engine gains its energy from heat released during the combustion of the nonreacted working fluids, the oxidizer-fuel mixture. This process occurs within the engine and is part of the thermodynamic cycle of the device. At first, the combustion chamber is filled with the reactants. Initially, the free-piston is in the bottom of the combustion chamber. Then, the compression-combustion-expansion cycle is initiated by injection of compressed air at a predefined pressure through the launch mechanism. As the free-piston moves up, at some point the charge self-combusts if enough energy is supplied, then the free-piston continues to move until the top dead center. Finally, the free-piston moves down again under the force of the compressed gasses in the combustion chamber. Here and after, bottom and top represented in Figure 1 along with moving up and down are the essential terms for engines. In addition, two different detection devices are used to monitor important parameters during the experiment. The high-speed video and motion analysis is used to capture visible heterogeneous and homogeneous combustion processes, and to determine the velocity and position of the free-piston. The maximum frame rate and temporal resolution of the high-speed video and motion analysis are 3.2 Gigapixels per second throughput and one microsecond, respectively. The high-speed video and motion analysis is triggered when the compressed air solenoid valve is actuated. The laser beam is irradiated to the plexiglass cylinder through a collimator lens, and used as the light source of high-speed video and motion analysis. Infrared thermal imager monitors the two-dimensional temperature distributions inside the combustion chamber of the engine. The initial pressures for all experiments are 0.1 MPa. In addition, the initial temperature is 300 K. All of the experimental results are presented from a series of experiments with fuel-lean methane-air mixtures.

Additionally, many fundamental and application studies have been carried out for hydrogen enrichment combustion in homogeneous charge compression ignition engines, using small amounts of hydrogen as additive to conventional hydrocarbon fuels [25]. Previous studies have shown that the hydrogen enrichment can not only improve ignition and combustion capabilities and engine efficiency, but also reduce emissions [26]. In addition, the self-ignition nature of hydrogen-air mixtures over platinum under very fuel-lean conditions offers an opportunity to self-ignite hydrocarbons with the assistance of small amounts of hydrogen [27], which can be reformed from hydrocarbons and is subsequently used for startup [28]. Therefore, it might be worthwhile to explore the feasibility of applying the technique of hydrogen enrichment or hydrogen assisted self-ignition of hydrocarbons to free-piston micro-engines, and, if feasible, to thoroughly study their combustion characteristics and engine performance in the purely homogeneous and coupled heterogeneous and homogeneous combustion modes.

3. Numerical methods

The characteristic length of the combustion chamber and the reacting gas flow path in micro-engines is still sufficiently larger than the molecular mean-free path of the air and other gases flowing through the system. Hence, the fluid can be reasonably considered as continuous and the Navier-Stokes equations are applicable to the present work. Simulations were performed using the initial parameters of the micro-engine used in the single-shot heterogeneous and homogeneous combustion experiments. In the physical system depicted in Figure 2, the upper surface of the free-piston and the lower surface of the end-plug were coated with a catalyst. The computational domain is a two-dimensional channel of initial length 20 mm and cylinder bore 3 mm, coupled with two gaps (between cylinder walls and free-piston) of length 6 mm (corresponding to the free-piston length) and various diameters. The thickness of the catalytic layer is several orders of magnitude smaller than the combustion chamber, so the effect of the catalyst volume can be neglected. A two-dimensional, viscous, compressible, and transient numerical model was used that includes detailed heterogeneous and homogeneous chemistry and transport, leakage, heat transfer, dynamic mesh, and thermodynamic-dynamic balance.

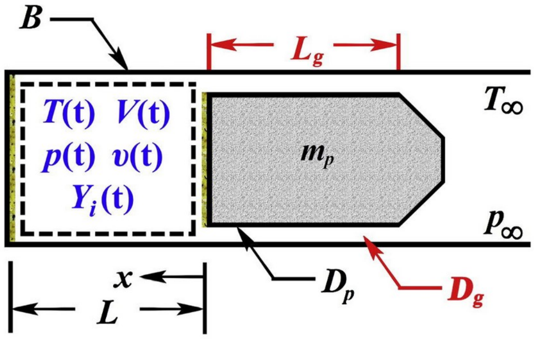


Figure 2. Schematic representation of the computational domain. The upper surface of the free-piston and the lower surface of the end-plug were coated with a catalyst.

The distinguishing feature of this free-piston micro-engine is a mechanically unconstrained piston. Consequently, reciprocating motion is the result of gas pressure acting on the free-piston, in contrast to a traditional crankshaft-equipped engine. Free-piston motion is the result of a thermodynamic-dynamic balance. Experimentations have demonstrated that the oscillation frequency of free-piston is determined by the average gas pressures and the free-piston mass. In order to solve the coupling problem of free-piston movement and heterogeneous and homogeneous combustion, we developed a dynamic mesh program of free-piston based on computational fluid dynamics software: FLUENT® Release 6.3, coupled with CHEMKIN. The dynamic mesh model of six degree of freedom and the mesh method of layering were used; and a User-Defined Function subroutine written in the C programming language was used to define the six degree of freedom parameters and to specify the boundary conditions of the free-piston motion. Computational fluid dynamics-based six degree of freedom simulations are based on evaluating the conservation equations for the fluid, such as the unsteady Reynolds-averaged Navier-Stokes equations, along with the motion equations for the solid. This approach can significantly simplify the dynamic mesh settings, in spite of the increased computational cost. Different gap sizes between cylinder walls and free-piston were used to examine the leakage effect. Compared with the experimental results, it is found that the gap size of 6 μm is appropriate. Finer mesh was used to discretize the gap in the transverse direction.

The gas-phase in the combustion chamber and the two gaps between cylinder walls and free-piston is described by the conservation equations for mass, energy, and momentum species. Therein, compressibility effects caused by density variations and heat release are fully considered; while acoustic waves are neglected, which allows for longer integration times steps. In addition, the mathematical model is developed by employing a force balance to the free-piston. Leakage, the gas escaping through the gap between cylinder walls and free-piston from combustion chamber, is described by two-dimensional transient-state compressible flow; this strategy is a necessity because we found that the pressure drop occurs in this gap is appreciable.

4. Results and discussion

Representative image sequences from the single-shot experiments in different combustion modes are presented in Figure 3. Both purely homogeneous and coupled heterogeneous and homogeneous combustion of methane in a narrow cylinder with a diameter of 3 mm and a height of approximately 0.3 mm are possible. It is noteworthy because the cylinder is neither heated nor insulated and the charge is initially at ambient conditions. Moreover, the free-piston near the top dead center of the compression stroke is virtually stationary during each combustion. As a result, purely homogeneous or coupled heterogeneous and homogeneous combustion is essentially a constant-volume process, as well as one would expect the fuel conversion efficiency to approach the Otto cycle limit if the whole charge is consumed and the heat transfer is negligible. Furthermore, Figure 3(a) demonstrates that homogeneous charge compression ignition at the micro-scale is capable of igniting methane-air mixtures that traditionally cannot be combusted. In addition, Figure 3(a) also reveals that ignition starts at the center of the combustion chamber, and that homogeneous charge compression ignition proceeds through localized homogeneous reactions although only part of the charge is consumed.

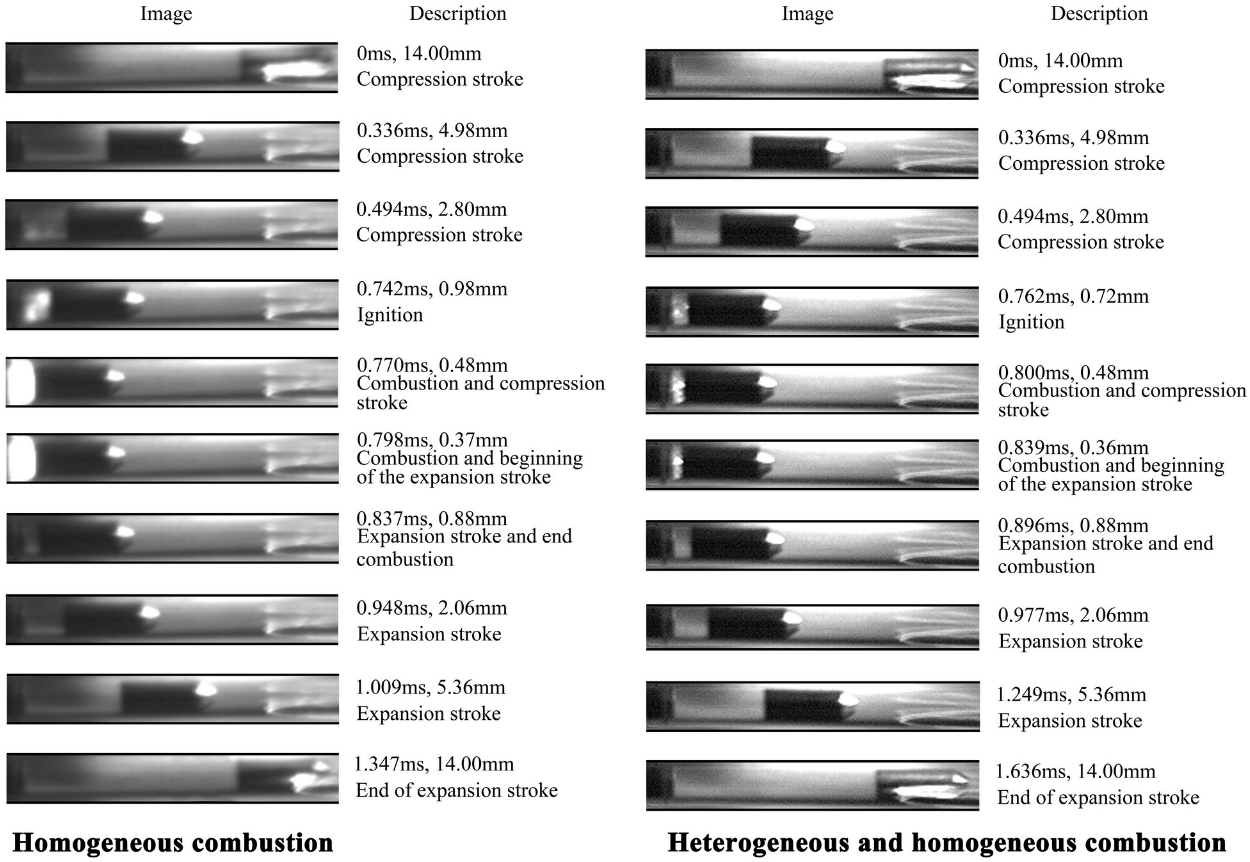
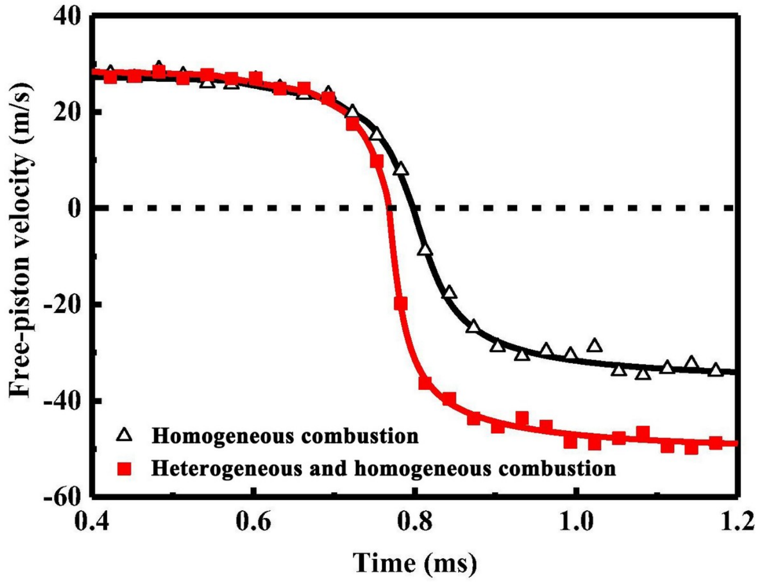


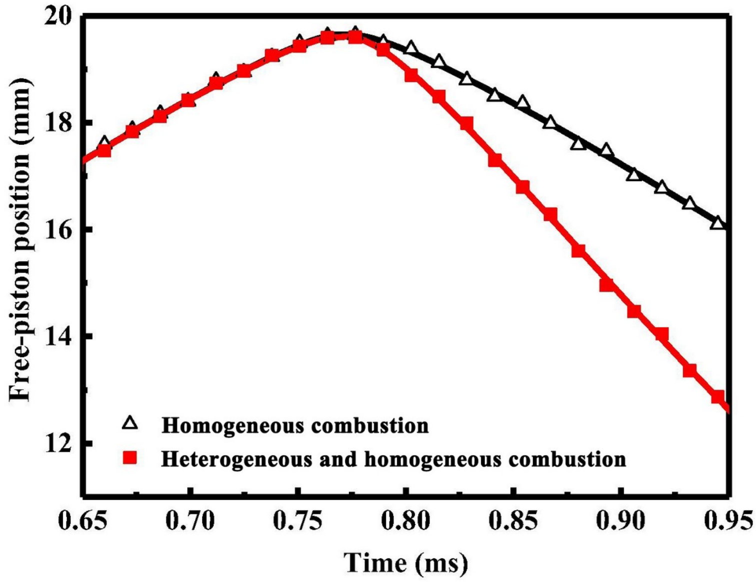
Figure 3. Typical image sequences from the single-shot experiments in different combustion modes. The fuel is methane and the charge is initially at ambient pressure and temperature.

Compared to the coupled heterogeneous and homogeneous combustion (Fig. 3(b)), the purely homogeneous flame (Fig. 3(a)) under non-catalytic conditions is very weak and accompanied by only part of the reactants is consumed, along with the significantly extended compression combustion expansion cycle as a result of its lower free-piston velocity during the expansion stroke. In the coupled heterogeneous and homogeneous combustion mode, heterogeneous reactions can significantly improve the fuel conversion efficiency and in-cylinder temperature and enhance combustion process, resulting in a shorter cycle period. In order to improve the power density and to achieve reliable auto-ignition, the micro-engine must operate at kilohertz frequencies, placing requirements about the allowable ignition delay times. In addition, the lower apparent activation energy of heterogeneous reaction causes earlier ignition, resulting in lower ignition temperature and pressure. Earlier ignition extends the reaction time inside the combustion chamber, and consequently improve the combustion efficiency, which is very favorable for the micro-device.

Experimental results of the free-piston dynamics in the purely homogeneous and coupled heterogeneous and homogeneous combustion modes are compared in Figure 4. For the compression path, two combustion modes give similar predictions of the free-piston velocity and position, but the expansion paths vary greatly. When the free-piston approaches the top dead center, the compression rate or the free-piston velocity slows down while the in-cylinder charge continues to leak through the gap between cylinder walls and free-piston from combustion chamber, at a rate that is proportional to the cylinder pressure. Then, the in-cylinder charge is ignited and, consequently, the in-cylinder temperature and pressure jump, associated with a sharp increase in the amount of charge loss. Near the ignition timing, the free-piston velocity varies rapidly. In addition, energy released by combustion results in higher free-piston velocity during the expansion stroke. Coupled heterogeneous and homogeneous combustion results in higher free-piston velocity during the expansion stroke. However, during the compression stroke, there is only marginal difference between the free-piston velocities obtained from different combustion modes. The free-piston motion profile differs from that of traditional engines, with the primary difference being a significantly higher piston acceleration around the top dead center [14]. Furthermore, the significantly shorter time spent around the top dead center in the coupled heterogeneous and homogeneous combustion mode are evident, compared to that in the purely homogeneous combustion mode.



(a) Free-piston velocity



(b) Free-piston position

Figure 4. A comparison of the measured free-piston velocities and positions between the purely homogeneous (black symbols) and coupled heterogeneous and homogeneous (red symbols) combustion modes.

To facilitate performance comparisons between the different combustion modes, the same simulation conditions were chosen. Comparisons are elaborated for the free-piston initial velocity of

30 meters per second. In the coupled heterogeneous and homogeneous combustion mode, two-dimensional temperature contours acquired from transient simulation at various points in time are provided in Figure 5. The corresponding temperature contours and average temperature profile in the purely homogeneous combustion mode are also shown in the same figures. Ignition is indicated by a sudden temperature rise. Clearly, the coupled heterogeneous and homogeneous combustion mode shows a completely different ignition behavior from that of the purely homogeneous case. The heterogeneous reaction initially causes a more rapid temperature rise and increases the overall reaction rate, resulting in a higher fuel conversion and a shorter ignition delay compared to the purely homogeneous case. Peak temperature and ignition timing are significantly affected by heterogeneous reaction with lower activation energy. The catalyst opens new reaction pathways, extending the range of reactivity toward lower temperatures as well as accelerating reactions at higher temperatures. In addition, in the coupled heterogeneous and homogeneous combustion mode, mass and heat loss causes exhaust temperatures to decrease faster during the expansion stroke.

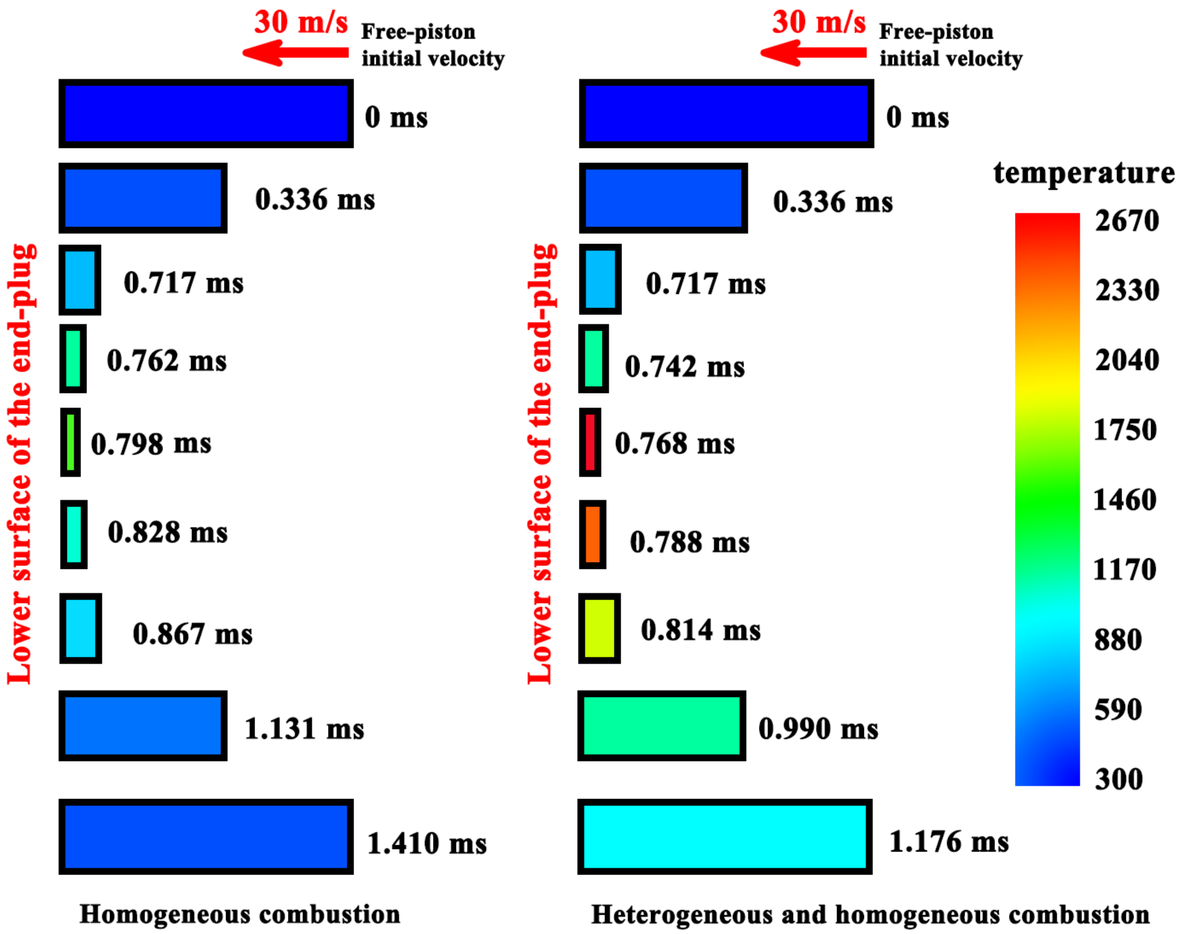


Figure 5. Predicted two-dimensional temperature contours at various points in time in different combustion modes.

Predicted two-dimensional temperature distributions at the top dead center in the coupled heterogeneous and homogeneous combustion mode are provided in Figure 6; the corresponding temperature distributions in the purely homogeneous case are also shown in the same figure. In the purely homogeneous combustion mode, the temperatures in the fluid region are almost identical and within the maximum difference of 8 K. However, in the coupled heterogeneous and homogeneous combustion mode, the highest temperature is found on the catalytic walls, i.e., the upper surface of the free-piston and the lower surface of the end-plug; it is also significantly higher than that in the purely homogeneous case. In addition, coupled heterogeneous and homogeneous combustion results in lower compression ratios than the purely homogeneous case and less time spent around the top dead center, as will be discussed in the free-piston dynamics section.

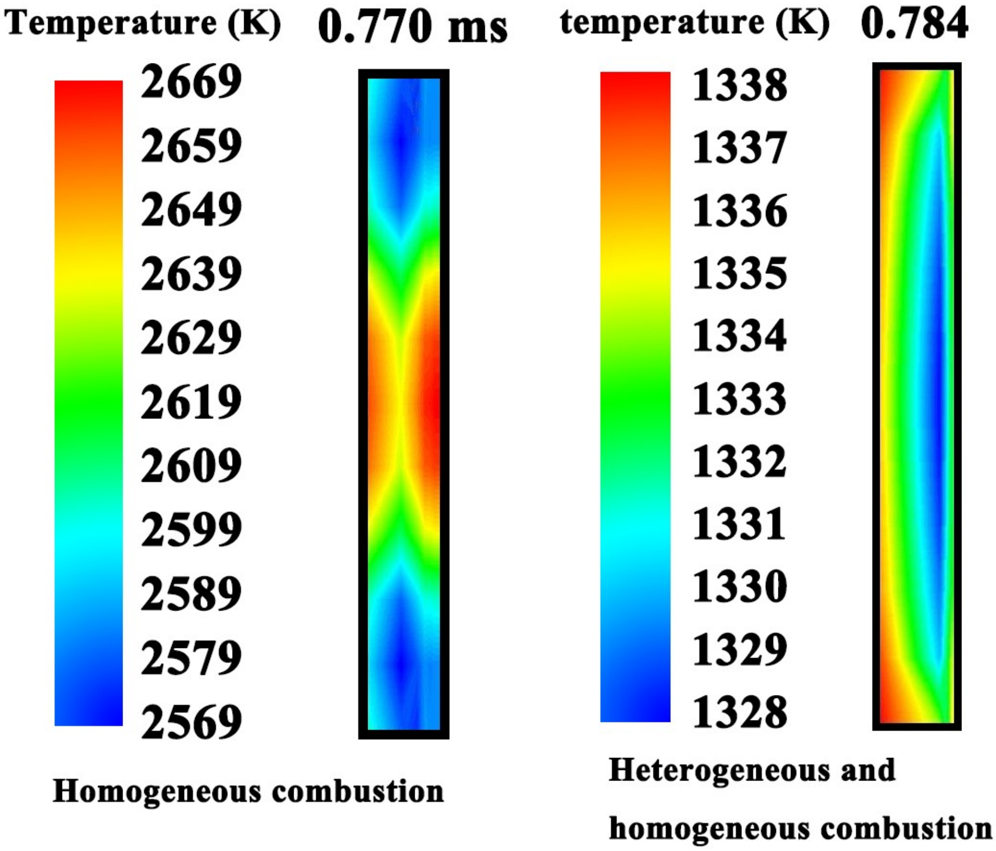


Figure 6. Predicted two-dimensional temperature distributions at the top dead center in different combustion modes.

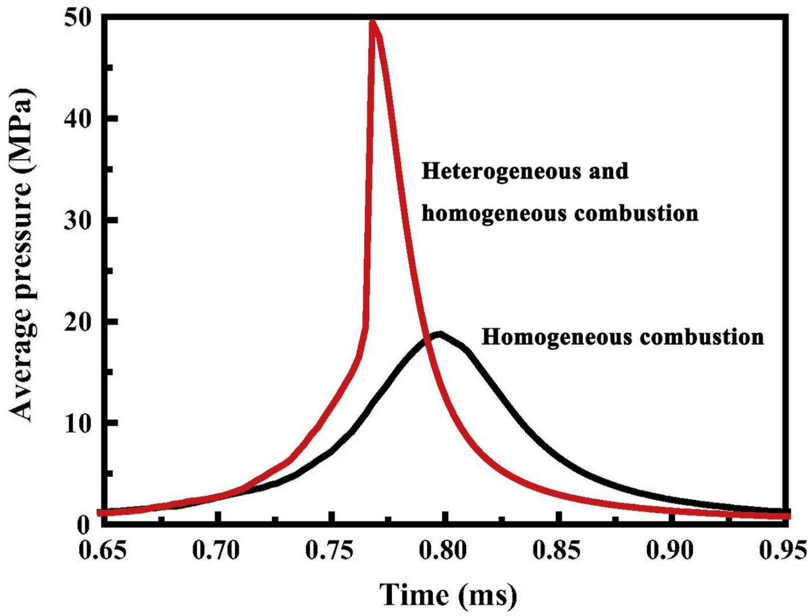
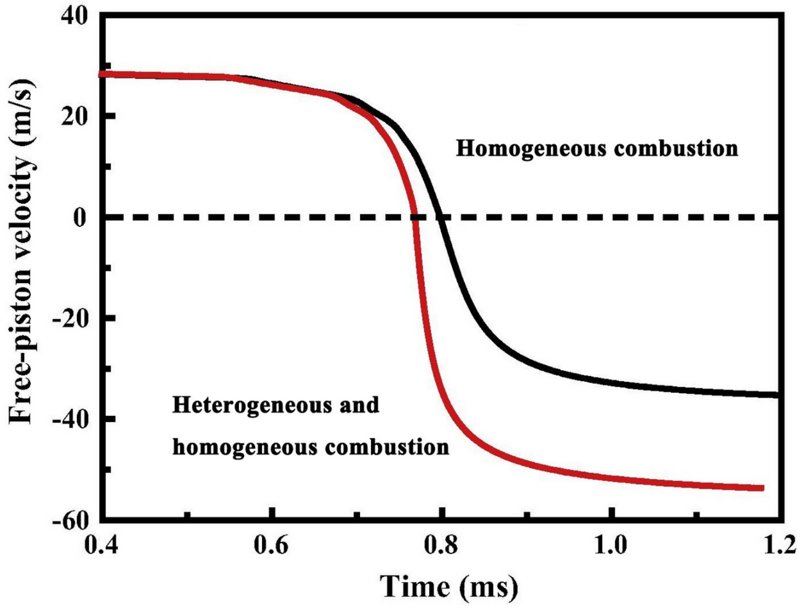
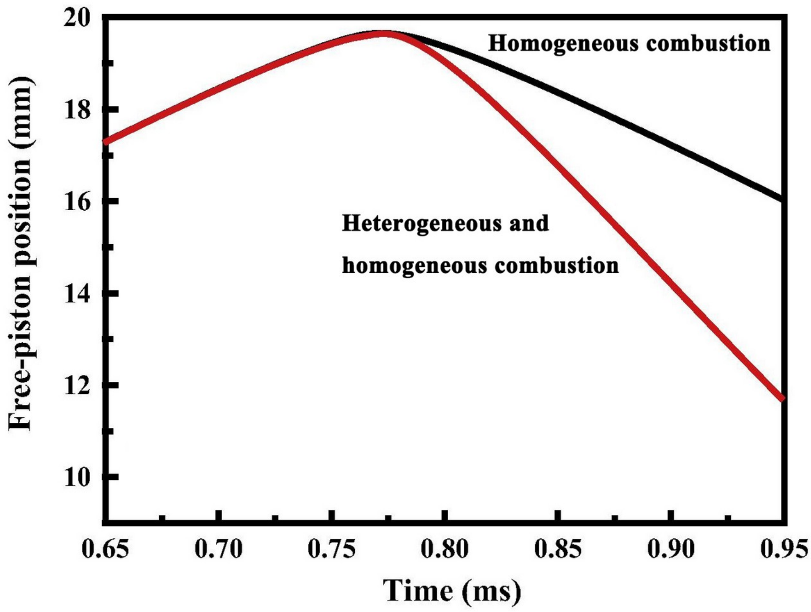


Figure 7. Predicted profiles of average pressure in different combustion modes. At first, in both combustion modes, the in-cylinder pressure grows because of compression. When the free-piston approaches the top dead center, the ignited in-cylinder charge results in a sharp increase in the in-cylinder pressure, irrespective of combustion mode.

The catalytic effect on the in-cylinder pressure is shown in Figure 7. At first, in both combustion modes, the in-cylinder pressure grows because of compression. When the free-piston approaches the top dead center, the ignited in-cylinder charge results in a sharp increase in the in-cylinder pressure, irrespective of combustion mode. During the expansion stroke, the in-cylinder pressure is sharply reduced because of the increase in the volume as well as the heat and mass loss. Coupled heterogeneous and homogeneous combustion results in significantly higher in-cylinder pressure and, consequently, higher mass loss rate; it also leads to an increase in the in-cylinder volume due to the higher free-piston velocity during the expansion stroke. These cause product pressure to decrease faster in the coupled heterogeneous and homogeneous combustion mode during the expansion stroke, even significantly lower than that in the purely homogeneous case in most of the expansion process. In addition, heterogeneous reaction results in earlier ignition and higher peak pressure.



(a) Free-piston velocity



(b) Free-piston position

Figure 8. A comparison of the predicted free-piston velocities and positions between the purely homogeneous (black lines) and coupled heterogeneous and homogeneous (red lines) combustion modes.

The predicted free-piston dynamics including the free-piston velocity and position in various combustion modes are compared in Figure 8. As observed, the position traces of free-piston in various combustion modes are identical during the compression stroke, but differ in the expansion stroke. Coupled heterogeneous and homogeneous combustion results in the significantly shorter time spent around the top dead center. For the compression path, two combustion modes give similar predictions of the free-piston dynamics, but the expansion paths vary greatly. This occurs because different fuel conversion efficiencies and mass losses occur when the free-piston reverses direction. When the free-piston approaches the top dead center, the free-piston velocity varies rapidly. During the expansion stroke, coupled heterogeneous and homogeneous combustion results in higher free-piston velocity, while the free-piston velocity in the purely homogeneous combustion mode is only slightly increased as a result of lower combustion efficiency as well as heat and mass loss. However, during the compression stroke, there is only marginal difference between the free-piston dynamics obtained from different combustion modes.

5. Conclusions

The heterogeneous and homogeneous combustion-based homogeneous charge compression ignition of fuel-lean methane-air mixtures over alumina-supported platinum catalysts in free-piston micro-engines was investigated experimentally and numerically. Single-shot experiments were carried out in free-piston micro-engines. In addition, a two-dimensional transient model with detailed chemistry and transport simulated the single-shot experiments to gain physical insight and to explore the heterogeneous and homogeneous combustion characteristics in free-piston micro-engines. Specific results are summarized as follows:

- Both purely homogeneous and coupled heterogeneous and homogeneous combustion of methane-air mixtures in a narrow cylinder with a diameter of 3 mm and a height of approximately 0.3 mm is possible, and methane at equivalence ratio of 0.8 is demonstrated in both cases.
- Coupled heterogeneous and homogeneous combustion reduces the mass loss because of its lower compression ratio as well as less time spent around the top dead centre and during the expansion stroke, whereas heat losses result in higher mass losses.
- Coupled heterogeneous and homogeneous combustion results in more complete fuel conversion and higher temperature and energy release, as well as significantly improves the output power and energy density.
- A two-dimensional transient numerical model which couples detailed heterogeneous and homogeneous chemistry and transport, leakage, heat transfer, and free-piston motion is developed, as well as used to model the single-shot experiments in free-piston micro-engines and to explore the heterogeneous and homogeneous combustion-based homogeneous charge compression ignition. This model approximates the single-shot process, and the model predictions are generally consistent with the experimental data.
- Heterogeneous reactions cause earlier ignition, reduce the ignition delay time, and consequently extend the reaction time. These are very favourable for the micro-device.
- In micro-scales, traditional engine combustion schemes are generally infeasible because of quenching effects and insufficient residence times, whereas the coupled heterogeneous and homogeneous combustion mode-based homogeneous charge compression ignition is a promising alternative.

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